

S-Methylpropanethiosulfonate

Other names:	Methyl propanethiosulfonate
Inchi:	InChI=1S/C4H10O2S2/c1-3-4-8(5,6)7-2/h3-4H2,1-2H3
InchiKey:	ZFMGGTVJCVKKJZ-UHFFFAOYSA-N
Formula:	C4H10O2S2
SMILES:	CCCS(=O)(=O)SC
Mol. weight [g/mol]:	154.25

Physical Properties

Property code	Value	Unit	Source
gf	-452.62	kJ/mol	Joback Method
hf	-537.37	kJ/mol	Joback Method
hfus	21.62	kJ/mol	Joback Method
hvap	49.95	kJ/mol	Joback Method
log10ws	-1.20		Crippen Method
logp	1.089		Crippen Method
mvol	111.660	ml/mol	McGowan Method
pc	4890.21	kPa	Joback Method
rinpol	1188.00		NIST Webbook
tb	407.48	K	Joback Method
tc	595.52	K	Joback Method
tf	207.80	K	Joback Method
vc	0.440	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.61	J/molxK	407.48	Joback Method
cpg	211.26	J/molxK	438.82	Joback Method
cpg	220.61	J/molxK	470.16	Joback Method
cpg	229.63	J/molxK	501.50	Joback Method
cpg	238.31	J/molxK	532.84	Joback Method
cpg	246.65	J/molxK	564.18	Joback Method
cpg	254.64	J/molxK	595.52	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U322289&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rlnol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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